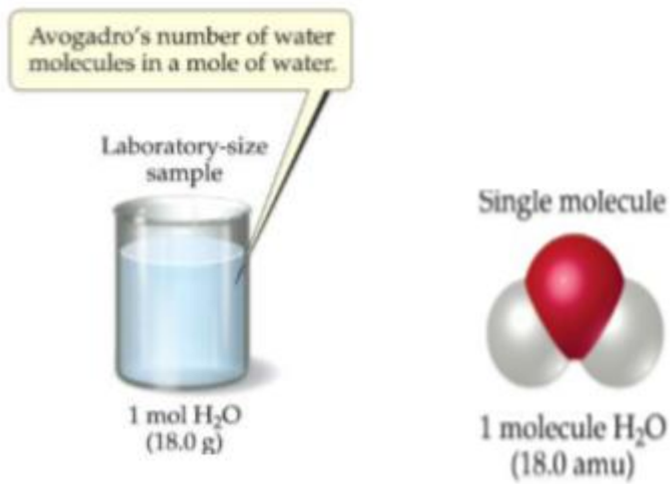
FARJANA YEASMIN
LECTURER, DEPT. OF FSE

CHEMICAL BALANCE & STOICHIOMETRY

Avogadro's Number and the Mole:

A mole is Avogadro's number of things. There are 6.022×10^{23} atoms in 12.00 g of 12C. The former quantity is known as Avogadro's number and is the basis for the SI unit of amount, the mole (mol): 1 mole = 6.022×10^{23}



Molar Mass

The mass in grams of 1 mole of substance is said to be the molar mass of that substance. Molar mass has units of g/mol. The mass of 1 mole of 12C = 12 g.

The molar mass of a molecule is the sum of the molar masses of the atoms:

Example: The molar mass of N_2 = 2 x (molar mass of N).

•Molar masses for elements are found on the periodic table.

•The formula weight (in amu) is numerically equal to the molar mass (in g/mol).

Molecular formula

The molecular formula is an expression of the number and type of atoms that are present in a single molecule of a substance. It represents the actual formula of a molecule. Subscripts after element symbols represent the number of atoms. If there is no subscript, it means one atom is present in the compound. For example, the molecular formula of glucose is $C_6H_{12}O_6$, which indicates that a molecule of glucose contains 6 atoms of carbon, 12 atoms of hydrogen, and 6 atoms of oxygen.

Empirical formula

Empirical formulas show which elements are present in a compound, with their mole ratios indicated as subscripts. For example, the empirical formula of glucose is CH_2O, which means that for every mole of carbon in the compound, there are 2 moles of hydrogen and one mole of oxygen.

Molecular weight

Molecular weight is the sum of the atomic weights of atoms in a molecule's molecular formula. Example: The molecular weight of the molecule ethane, C_2H_6, would be calculated as follows:

C= 2(12.01 amu) = 24.02 amu C

H= 6(1.01 amu) = 6.06 amu H

So, total molecular weight of ethane= (24.02+ 6.06)=30.08 amu C_2H_6

Formula weight

Formula weight is the sum of the atomic weights of the atoms in a molecule's empirical formula. Example: The formula weight of the empirical ethane, CH_3, would be calculated as follows:

C= 1(12.01 amu) = 12.01 amu C

H= 3(1.01 amu) = 3.03 amu H

So, total formula weight of ethane= (12.01 + 3.03)=15.04 amu CH_3

Determining Percent Composition Based on the Chemical Formula of a Compound

When a compound's formula is unknown, measuring the mass of each of its constituent elements is often the first step in the process of determining the formula experimentally.

Example 1: Analysis of a 12.04g sample of a liquid compound composed of carbon, hydrogen, and nitrogen showed it to contain 7.34 g C, 1.85 g H, and 2.85 g N. What is the percent composition of this compound?

Solution: To calculate percent composition, we divide the experimentally derived mass of each element by the overall mass of the compound, and then convert to a percentage:

$$\%\,\mathrm{C} = \frac{7.34\ g\ C}{(12.04\ \mathrm{g\ compound})} \times 100 = 61.0\%$$

$$\%\,\mathrm{H} = \frac{1.85\ g\ C}{(12.04\ \mathrm{g\ compound})} \times 100 = 15.4\%$$

$$\%\,\mathrm{N} = \frac{2.85\ g\ C}{(12.04\ \mathrm{g\ compound})} \times 100 = 23.7\%$$

CHEMICAL BALANCE & STOICHIOMETRY

The analysis results indicate that the compound is 61.0% C, 15.4% H, and 23.7% N by mass.

Example 2: Determine the mass-percentage of carbon in ethane (C_2H_6). (MW of ethane = 30.08 amu)

$$\%\ \text{Element} = \frac{(\text{number of atoms in formula})\ (\text{atomic weight})}{(\text{MW of the compound})} \times 100$$

$$\text{So}, \%\ \text{C} = \frac{(2)(12.01\ amu)}{(30.08\ \text{amu})} \times\ 100 = 79.85\%$$

Empirical Formula Calculation Steps

Step 1: If you have masses go onto step 2. But if you have %. Assume the mass to be 100g, so the % becomes grams.

Step 2: Determine the moles of each element.

Step 3: Determine the mole ratio by dividing each elements number of moles by the smallest value from step 2.

Step 4: Double, triple … to get an integer if they are not all whole numbers

CHEMICAL BALANCE & STOICHIOMETRY

Molecular Formula (additional steps)

***The question should have included a molecular mass.

Step 5: Determine the mass of your empirical formula

Step 6: Divide the given molecular mass by your E.F. mass in step 5

Step 7: Multiply the atoms in the empirical formula by this number

Examples-Caffeine has an elemental analysis of 49.48% carbon, 5.190% hydrogen, 16.47% oxygen, and 28.85% nitrogen. It has a molar mass of 194.19 g/mol. What is the molecular formula of caffeine?

Given: 49.48% C, 5.190%H, 16.47% O and 28.85% N

Step 1: Assume a mass of 100g so % becomes grams

49.48g C, 5.190gH, 16.47g O and 28.85g N

Step 2: determine the moles of each element

49.48g C x (1 mole/12.0 g C) = 4.123moles C
5.190g H x (1 mole / 1.0 g H) = 5.190 moles H
16.47g O x (1 mole /16.0 g O) =1.029moles O

28.85g N x (1 mole/ 14.0 g N) = 2.061 moles N

Step 3: determine the mole ratio by dividing each elements number of moles by the smallest

Dividing by the smallest (1.029) we get

C: 4.123 / 1.029 = 4.007
H: 5.190 / 1.029 = 5.044
O: 1.029 / 1.029 =1.000
N: 2.061 / 1.029 = 2.002

Step 4 : Double, triple .. to get an integer is they are not all whole numbers

The values are all really close to whole numbers.

Empirical Formula= $\mathbf{C_4H_5ON_2}$

Example- Molecular Formulas (Steps 5-7)

It has a molar mass of 194.19 g/mol.(given)

Step 5: After you determine the empirical formula, determine its mass.

Empirical Formula= $C_4H_5ON_2$

(4 carbon x 12.0) + (5 hydrogen x1.0) + (1 oxygen x 16.0) + (2 nitrogen x 14.0) =97.0g/mol

Step 6: Determine how many times greater the molecular mass is compared to the mass of the empirical formula.

molecular mass/ empirical formulas mass

194.19g/mol / 97.0g/mol = 2

Step 7 :Multiply the empirical formula by this number

2x $C_4H_5ON_2$=$\mathbf{C_8H_{10}O_2N_4}$

better==> $C_8H_{10}N_4O_2$

CHEMICAL BALANCE & STOICHIOMETRY

Classifying Chemical Reactions

Many reactions fall into one of the following three categories:

1. Combination reactions
2. Decomposition reactions
3. Combustion reactions

Combination (or Synthesis) Reaction

Two or more substances react to form one product. Some examples:

$$N_2(g) + 3\ H_2(g) \rightarrow 2\ NH_3(g)$$

$$C_3H_6(g) + Br_2(l) \rightarrow C_3H_6Br_2(l)$$

Decomposition Reaction

One substance breaks down into two or more substances. Some examples:

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

$$2\ KClO_3(s) \rightarrow 2\ KCl(s) + O_2(g)$$

Combustion Reactions

This reactions are generally rapid reactions that produce flames. Most involve oxygen (from the air) as a reactant. Also involve a fuel that reacts with O_2 to form one or more oxidized products.

Some examples of hydrocarbon combustion. Complete combustion of hydrocarbon fuels results in the products CO_2 and H_2O.

$$CH_4(g) + 2\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(g)$$

$$C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(g)$$

FARJANA YEASMIN
LECTURER, DEPT. OF FSE

CHEMICAL BALANCE & STOICHIOMETRY

Balancing Equations

Matter cannot be lost in any chemical reaction. Therefore, the products of a chemical reaction have to account for all the atoms present in the reactants. So, we must balance the chemical equation.

When balancing a chemical equation we adjust the stoichiometric coefficients in front of chemical formulas. Subscripts in a formula are never changed when balancing an equation.

Example: the reaction of methane with oxygen:

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

•Counting atoms in the reactants yields: 1 C; 4 H; and 2 O.

•In the products we see: 1 C; 2 H; and 3 O.

•It appears as though an H has been lost and an O has been created.

•To balance the equation, we adjust the stoichiometric coefficients:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

Indicating the States of Reactants and Products

The physical state of each reactant and product may be added to the equation:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

Reaction conditions may appear above or below the reaction arrow (e.g., "Δ" is used to indicate the addition of heat).

FARJANA YEASMIN
LECTURER, DEPT. OF FSE

CHEMICAL BALANCE & STOICHIOMETRY

Stoichiometry

Stoichiometry is the study of the quantitative aspects of chemical formulas and chemical reactions or the mass relationships in chemistry. Based on the Law of Conservation of Mass (Antoine Lavoisier, 1789), as explained by the Atomic Theory of Matter (John Dalton, 1800). Using a balanced chemical equation to calculate amounts of reactants and products is called stoichiometry.

Stoichiometry problem : For the following *unbalanced* reaction, how many grams of NaOH will be required to fully react with 3.10 grams of H_2SO_4?

$NaOH(aq) + H_2SO_4\ (aq) \rightarrow H_2O + Na_2SO_4(aq)$ Not balanced!

For this reaction, we have 1 Na and 3 H on the reactant side and 2 Na and 2 H on the product side. We can balance our equation by multiplying NaOH by two—so that there are 2 Na on each side—and multiplying H2O by two—so there are 6 O and 4 H on both sides. That gives the following balanced reaction:

$$2NaOH(aq) + H_2SO_4\ (aq) \rightarrow 2H_2O + Na_2SO_4(aq)$$

Once we have the balanced equation, we can ask ourselves the following questions:

- For which reactant(s) do we already know the amount of the chemical?
- What are we trying to calculate?

In this example, we know the amount of H_2SO_4 is 3.10 grams, and we would like to calculate the mass of NaOH. So armed with the balanced equation we can use the following strategy to tackle this stoichiometry problem:

CHEMICAL BALANCE & STOICHIOMETRY

Step 1: Convert known reactant amount to moles.

The known quantity in this problem is the mass of H_2SO_4. We can convert the mass of H_2SO_4 to moles using the molecular weight. Given that the molecular weight of H_2SO_4 is 98.09 g/mol, we can find the moles of H_2SO_4 as follows:

$$3.10\ \cancel{\mathrm{g\,H_2SO_4}} \times \frac{1\,\mathrm{mol\,H_2SO_4}}{98.09\ \cancel{\mathrm{g\,H_2SO_4}}} = 3.16 \times 10^{-2}\mathrm{mol\,H_2SO_4}$$

Step 2: Use mole ratio to find moles of other reactant.

We are interested in calculating the amount of NaOH, so we can use the mole ratio between NaOH and H_2SO_4. Based on our balanced chemical equation, we need 2 moles of NaOH for every 1 mole of H_2SO_4, which gives the following ratio:

$$\text{Mole ratio between NaOH and } \mathrm{H_2SO_4} = \frac{2\,\mathrm{mol\,NaOH}}{1\,\mathrm{mol\,H_2SO_4}}$$

We can use the ratio to convert moles of H_2SO_4 from step one to moles of NaOH:

$$3.16 \times 10^{-2}\ \cancel{\mathrm{mol\,H_2SO_4}} \times \frac{2\,\mathrm{mol\,NaOH}}{1\ \cancel{\mathrm{mol\,H_2SO_4}}} = 6.32 \times 10^{-2}\,\mathrm{mol}$$

CHEMICAL BALANCE & STOICHIOMETRY

Step 3: Convert moles to mass.

We can convert the moles of NaOH from Step 2 to mass in grams using the molecular weight of NaOH:

$$6.32 \times 10^{-2} \cancel{\text{mol NaOH}} \times \frac{40.00\,\text{g NaOH}}{1\,\cancel{\text{mol NaOH}}} = 2.53\,\text{g NaOH}$$

We will need 2.53 grams of NaOH **to fully react with 3.10 grams of** H_2SO_4 **in this reaction.**

Limiting Reactants

It is not necessary to have all reactants present in stoichiometric amounts. Often, one or more reactants is present in excess. Therefore, at the end of reaction those reactants present in excess will still be in the reaction mixture. The reactants that are completely consumed are called the limiting reactants or limiting reagents. Reactants present in excess are excess reactants or excess reagents.

Consider 10 H_2 molecules mixed with 7 O_2 molecules to form water. The balanced chemical equation tells us that the stoichiometric ratio of H_2 to O_2 is 2 to 1:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$

CHEMICAL BALANCE & STOICHIOMETRY

•This means that our 10 H_2 molecules require 5 O_2 molecules (2:1). Since we have 7 O_2 molecules, our reaction is limited by the amount of H_2 we have. (the O_2 is in excess).

•So, all 10 H_2 molecules can (and do) react with 5 of the O_2 molecules producing 10 H_2O molecules.

•At the end of the reaction, 2 O_2 molecules remain unreacted.

Theoretical Yields

The amount of product predicted from stoichiometry, accounting for limiting reagents, is called the theoretical yield. This is often different from the actual yield -- the amount of product actually obtained in the reaction. The percent yield relates the actual yield (amount of material recovered in the lab) to the theoretical yield:

$$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$